

CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME II

Editors:

Ibrahim Ali Noorbatcha
Hamzah Mohd. Salleh
Mohamed Elwathig Saeed Mirghani
Raha Ahmad Raus



IIUM PRESS

INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA

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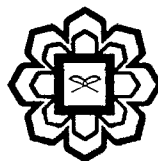
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IIUM Press

Published by:
IIUM Press
International Islamic University Malaysia

First Edition, 2011
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Perpustakaan Negara Malaysia

Cataloguing-in-Publication Data

Ibrahim Ali Noorbatcha, Hamzah Mohd. Salleh, Mohamed Elwathig Saeed Mirghani & Raha
Ahmad Raus: Current Research and Development in Biotechnology engineering at IIUM
Volume II

ISBN: 978-967-418-151-2

Member of Majlis Penerbitan Ilmiah Malaysia – MAPIM
(Malaysian Scholarly Publishing Council)

Printed by :
IIUM PRINTING SDN. BHD.
No. 1, Jalan Industri Batu Caves 1/3
Taman Perindustrian Batu Caves
Batu Caves Centre Point
68100 Batu Caves
Selangor Darul Ehsan

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MOLECULAR INTERACTION ANALYSIS TO DESIGN NEW DRUG CANDIDATES FOR LYSOSOMAL STORAGE DISEASE

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ABSTRACT

Acid β -glucosidase (GlcCerase) is a lysosomal enzyme, which is important in biodegradation of blood cells in human body. Mutation of GlcCerase will lead to Gaucher disease; the most common lysosomal storage disease. The current available treatments for gaucher disease are enzyme replacement therapy and substrate reduction therapy; and both are costly. New drugs for gaucher disease can be designed with the help of computer molecular modeling. A computational investigation of the active site of the GlcCerase using molecular docking approach leading to a better understanding of the drug action and suggesting new drugs for Gaucher disease is reported in this work.

Keywords: Gaucher disease, substrate reduction therapy, ligand design

INTRODUCTION

Gaucher disease is the most common lysosomal storage disorder. A deficiency of the enzyme glucocerebrosidase causes accumulation of the glycolipid glucocerebroside in macrophages throughout the body (Beutler, and Grabowski, 2001). In the viscera, glucocerebroside arises mainly from the biodegradation of red and white blood cells. In the brain, glucocerebroside arises from the turnover of complex lipids during brain development and the formation of the myelin sheath of nerves. The disease may be discovered as an incidental finding in the elderly because of mild thrombocytopenia or splenomegaly, or it may present early in life with hepatosplenomegaly, thrombocytopenia, anemia, and bone lesions

Gaucher disease has three common clinical subtypes. Type 1 is the most common form of the disease. It occurs most often among persons of Ashkenazi Jewish heritage (Dvir et al., 2003). Symptoms may begin early in life or in adulthood and include enlarged liver and grossly enlarged spleen, which can rupture and cause additional complications. Skeletal weakness and bone disease may be extensive. The brain is not affected, but there may be lung and, rarely, kidney impairment (Beutler, 2004). Patients in this group usually bruise easily and experience fatigue